Geoderma, 62 (1994) 83–92
Elsevier Science B.V., Amsterdam

Cokriging versus kriging in regionalized multivariate data analysis

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(Received July 20, 1992; accepted after revision May 18, 1993)

ABSTRACT

Cokriging and kriging are compared in the case when all variables are available at the same sample locations. The advantage of cokriging over kriging is that it ensures the coherence between an estimation of a sum and the separate estimation of each of its terms. To spare modeling effort it is interesting to know in which situation the kriging of a variable is equivalent to its cokriging with respect to a set of auxiliary variables (autokrigeability).

In regionalized multivariate data analysis (MDA) it is important to know whether a whole set of variables is autokrigeable (intrinsically correlated). Intrinsic correlation implies that underlying factors can be computed from a classical MDA instead of a coregionalization analysis and that they can be kriged instead of being cokriged. Three criteria for identifying intrinsic correlation are discussed.

INTRODUCTION

Kriging is a method to estimate, in a spatial context, the value of a variable of interest at a location where it has not been measured, using data in the neighborhood. Cokriging is the extension of kriging to the situation when auxiliary variables can be used to improve the accuracy of the kriging estimate.

When considering cokriging it is important to examine separately the *isotopic* case (from the Greek: *iso*=same and *topos*=location), where all variables have been measured at the same sample locations x_α, $\alpha=1, ..., n$ and the *heterotopic* case, where some sample locations are not shared by all variables. The heterotopic case, where the variable of interest is undersampled, has been extensively analyzed in the literature and numerous case studies show the benefits of taking into account the information provided by auxiliary variables correlated with the variable of interest.

In this article we restrict attention to the isotopic case and first treat the idea of coherence of the estimated values of a sum of variables, providing two examples. We remind the reader the equations of simple cokriging in compact matrix notation to show why cokriging is equivalent to kriging when the direct variogram is proportional to the cross variograms (autokrigeability) or

SSDI 0016-7061(93)E0065-4

when all the direct and cross variograms are proportional to a basic variogram model (intrinsic correlation). We transpose these concepts to regionalized multivariate data analysis (MDA) in the framework of the linear model of coregionalization and discuss, before concluding, several criteria for determining whether a coregionalization is intrinsically correlated.

COHERENCE

In the isotopic case the main advantage of cokriging versus kriging can be seen in the fact that the cokriging estimator of a sum of variables $S(\boldsymbol{x})$:

$$S(\boldsymbol{x}) = \sum_{i=1}^{N} Z_i(\boldsymbol{x}) \tag{1}$$

is *coherent* with the cokriging of the N terms $Z_i(\boldsymbol{x})$:

$$S^{\mathrm{CK}}(\boldsymbol{x}) = \sum_{i=1}^{N} Z_i^{\mathrm{CK}}(\boldsymbol{x}) \tag{2}$$

However, in general the kriging of $S(\boldsymbol{x})$ is not equal to the sum of the separate krigings of the $Z_i(\boldsymbol{x})$. We shall illustrate this with two examples (borrowed from Rivoirard, 1990).

Example 1: thickness of a soil horizon

The thickness $T(\boldsymbol{x})$ of a soil horizon is defined as the difference between its upper limit $Z_{\mathrm{U}}(\boldsymbol{x})$ and its lower limit $Z_{\mathrm{L}}(\boldsymbol{x})$:

$$T(\boldsymbol{x}) = Z_{\mathrm{U}}(\boldsymbol{x}) - Z_{\mathrm{L}}(\boldsymbol{x}) \tag{3}$$

Then, cokriging the thickness $T(\boldsymbol{x})$ using either $Z_{\mathrm{U}}(\boldsymbol{x})$ or $Z_{\mathrm{L}}(\boldsymbol{x})$ as an auxiliary variable is equivalent to taking the difference between the cokriged values of $Z_{\mathrm{U}}(\boldsymbol{x})$ and $Z_{\mathrm{L}}(\boldsymbol{x})$:

$$T^{\mathrm{CK}}(\boldsymbol{x}) = Z_{\mathrm{U}}^{\mathrm{CK}}(\boldsymbol{x}) - Z_{\mathrm{L}}^{\mathrm{CK}}(\boldsymbol{x}) \tag{4}$$

In general the kriging of the left-hand side is not coherent with the difference between the krigings of the right-hand side terms:

$$T^{\mathrm{K}}(\boldsymbol{x}) \neq Z_{\mathrm{U}}^{\mathrm{K}}(\boldsymbol{x}) - Z_{\mathrm{L}}^{\mathrm{K}}(\boldsymbol{x}) \tag{5}$$

and it cannot be decided which side of the equation yields the better estimated value for the thickness.

It should be noted that neither kriging nor cokriging will ensure a positive estimated value, a point that has been examined at length by Chauvet (1988).

Example 2: indicators of a discrete variable

Say we have data of a variable $Z(\boldsymbol{x})$ with four possible values:

$$\{0, 1, 2, 3\} \tag{6}$$

An indicator I_{cond} is a variable taking the value 1 if the condition *cond* is fulfilled, and the value 0 else. Obviously the cumulative indicator showing if $Z(\boldsymbol{x})$ is greater than (or equal to) 2 can be defined as the sum of the disjunctive indicators of $Z(\boldsymbol{x})$ for 2 and 3:

$$I_{Z(\boldsymbol{x})\geq 2} = I_{Z(\boldsymbol{x})=2} + I_{Z(\boldsymbol{x})=3} \tag{7}$$

and the cokriging of the cumulative indicator using one of the disjunctive indicators as an auxiliary variable is equal to the sum of the cokrigings of each disjunctive indicator.

But, except for what is called the *mosaic model*, the kriging of the cumulative indicator is not compatible with the sum of the krigings of the two disjunctive indicators:

$$I^{\mathrm{K}}_{Z(\boldsymbol{x})\geq 2} \neq I^{\mathrm{K}}_{Z(\boldsymbol{x})=2} + I^{\mathrm{K}}_{Z(\boldsymbol{x})=3} \tag{8}$$

This concept of coherence in the estimation of indicators is at the heart of a current debate about non-linear methods in geostatistics (e.g. see Lajaunie, 1992).

SIMPLE COKRIGING

When is cokriging equivalent to kriging in the isotopic case?

To examine this question we shall consider only *simple cokriging*, i.e. cokriging without any constraints on the weights, which implies second order stationarity and the existence of a cross covariance function $C_{ij}(\boldsymbol{h})$. The set of variograms $\gamma_{ij}(\boldsymbol{h})$ cannot be used for simple cokriging because it is a *conditionally* negative definite function and is appropriate only for kriging systems constraining the sum of weights to 0 or 1 for each variable.

The variable of interest in the set of variables $Z_i(\boldsymbol{x})$, $i = 1, \ldots, N$ is denoted by the index i_0. The simple cokriging estimator builds on the mean m_{i0} of the variable of interest, to which is added a sum of weights w^i_α, each multiplied by the difference of a sample $Z_i(\boldsymbol{x}_\alpha)$ with respect to the mean m_i:

$$Z^*_{i0}(\boldsymbol{x}_0) = m_{i0} + \sum_{i=1}^{N} \sum_{\alpha=1}^{n} w^i_\alpha \, (Z_i(\boldsymbol{x}_\alpha) - m_i) \tag{9}$$

By minimizing the variance of the estimation error between the unknown value $Z_{i0}(\boldsymbol{x}_0)$ and the estimator $Z^*_{i0}(\boldsymbol{x}_0)$ the following system is obtained in block matrix form:

$$\begin{pmatrix} C_{11} & \cdots & C_{1j} & \cdots & C_{1N} \\ \vdots & & & & \vdots \\ C_{i1} & & C_{ij} & & C_{iN} \\ \vdots & & & & \vdots \\ C_{N1} & \cdots & C_{Nj} & \cdots & C_{NN} \end{pmatrix} \begin{pmatrix} \boldsymbol{w}_1 \\ \vdots \\ \boldsymbol{w}_i \\ \vdots \\ \boldsymbol{w}_N \end{pmatrix} = \begin{pmatrix} \boldsymbol{c}_{1i_0} \\ \vdots \\ \boldsymbol{c}_{ii_0} \\ \vdots \\ \boldsymbol{c}_{Ni_0} \end{pmatrix} \tag{10}$$

where $\boldsymbol{C}_{ij}$ is the matrix of covariances between samples for the variable pair $\{Z_i, Z_j\}$, $\boldsymbol{w}_i$ is the vector of cokriging weights for the samples of the variable Z_i and $\boldsymbol{c}_{ii_0}$ is the vector of covariances between the sample locations $\boldsymbol{x}_\alpha$ and the location of interest $\boldsymbol{x}_0$ for the variable pair $\{Z_i, Z_{i_0}\}$.

AUTOKRIGEABILITY

A variable of interest is said to be *autokrigeable* (self-krigeable) with respect to a set of auxiliary variables if its cokriging is equivalent to its kriging. Matheron (1979) has shown that the variable of interest is autokrigeable when its cross variograms are proportional to its direct variogram:

$$\gamma_{i_0 j}(\boldsymbol{h}) = a_{i_0 j}\, \gamma_{i_0 i_0}(\boldsymbol{h}) \tag{11}$$

where $a_{i_0 j}$ are coefficients of proportionality. When covariances are used, this implies the same type of relationship:

$$C_{i_0 j}(\boldsymbol{h}) = a_{i_0 j}\, C_{i_0 i_0}(\boldsymbol{h}) \tag{12}$$

It is easy to check the autokrigeability for simple cokriging. Supposing, without loss of generality, that the first variable is the variable of interest, we obtain:

$$\begin{pmatrix} a_{11} \boldsymbol{C}_{ii} & \cdots & a_{1j} \boldsymbol{C}_{11} & \cdots & a_{1N} \boldsymbol{C}_{11} \\ \vdots & \ddots & & & \vdots \\ a_{i1} \boldsymbol{C}_{11} & & \boldsymbol{C}_{ij} & & \boldsymbol{C}_{iN} \\ \vdots & & & \ddots & \vdots \\ a_{N1} \boldsymbol{C}_{11} & \cdots & \boldsymbol{C}_{Nj} & \cdots & \boldsymbol{C}_{NN} \end{pmatrix} \begin{pmatrix} \boldsymbol{w}_1 \\ \vdots \\ \boldsymbol{w}_i \\ \vdots \\ \boldsymbol{w}_N \end{pmatrix} = \begin{pmatrix} a_{11} \boldsymbol{c}_{11} \\ \vdots \\ a_{i1} \boldsymbol{c}_{11} \\ \vdots \\ a_{N1} \boldsymbol{c}_{11} \end{pmatrix} \tag{13}$$

Obviously the vector $(\boldsymbol{w}_1, 0, \ldots, 0)^{\mathrm{T}}$, in which only the cokriging weights for the first variable are non zero, is a solution of the cokriging system. It is the unique solution as the system is assumed to be nondegenerate.

INTRINSIC CORRELATION

A set of variables is said to be *intrinsically correlated* if all direct and cross variograms are proportional by coefficients b_{ij} to a basic structure $\gamma(\boldsymbol{h})$:

$$\gamma_{ij}(\boldsymbol{h}) = b_{ij}\, \gamma(\boldsymbol{h}) \tag{14}$$

Similarly, in terms of covariance functions intrinsic correlation implies the model:

$$C_{ij}(\boldsymbol{h}) = \sigma_{ij}\,\rho(\boldsymbol{h}) \tag{15}$$

where σ_{ij} are the covariances between the variables and $\rho(\boldsymbol{h})$ is a spatial correlation function.

For a set of intrinsically correlated variables the isotopic simple cokriging can be written in compact form using the Kronecker product $\otimes$ (see e.g. Magnus and Neudecker, 1988):

$$(\boldsymbol{V} \otimes \boldsymbol{R})\boldsymbol{w} = \boldsymbol{v}_{i0} \otimes \boldsymbol{r}_{i0} \tag{16}$$

where $\boldsymbol{V}$ is the variance-covariance matrix, containing the covariances σ_{ij} between the variables; $\boldsymbol{R}$ is the spatial correlation matrix of the simple kriging system of the variable of interest; $\boldsymbol{w}$ is the vector of cokriging weights; $\boldsymbol{v}_{i0}$ is the column vector of $\boldsymbol{V}$ containing the covariances σ_{ii0} with the variable of interest; $\boldsymbol{r}_{i0}$ is the (rescaled) right-hand side of the simple kriging system of the variable of interest.

The vector $\boldsymbol{v}_{i0}$ on the right-hand side is a column of $\boldsymbol{V}$ on the left-hand side. Thus in the left-hand covariance matrix of the simple cokriging there is one column of matrices $\boldsymbol{R}$, each of which is multiplied by a different element of the vector $\boldsymbol{v}_{i0}$. Understanding this, it is now trivial that a vector $\boldsymbol{w}_{i0}$, defined as the only non zero subvector of $\boldsymbol{w}$ and containing the simple kriging weights for the samples of the variable of interest, represents the solution of the simple cokriging system for an intrinsically correlated coregionalization:

$$\begin{pmatrix} \\ \ldots\ \boldsymbol{v}_{i0} \otimes \boldsymbol{R}\ \ldots \\ \\ \end{pmatrix} \begin{pmatrix} 0 \\ \vdots \\ \boldsymbol{w}_{i0} \\ \vdots \\ 0 \end{pmatrix} = \boldsymbol{v}_{i0} \otimes \boldsymbol{r}_{i0} \tag{17}$$

Clearly, each of a set of intrinsically correlated regionalized variables is, by definition, autokrigeable. However, it is interesting to note that if a variable of interest is autokrigeable, this does not imply that the set of auxiliary variables is intrinsically correlated. Rivoirard (1989) has used this fact in nonlinear geostatistics to develop models based on orthogonal indicator residuals.

The concept of autokrigeability for the variable of interest or for a whole set of variables (in the case of intrinsic correlation) is also valid for ordinary cokriging with a variogram model.

INTRINSIC CORRELATION AND THE LINEAR MODEL

In this section we first discuss the implications of intrinsic correlation in a regionalized MDA based on the *linear model of coregionalization*. Then we consider the reverse: applying a classical MDA to spatial data which is not intrinsically correlated, and examine some of the consequences.

In the linear model of coregionalization the variables $Z_i(\boldsymbol{x})$ are represented as a linear combination of *uncorrelated* variables $Y_p^u(\boldsymbol{x})$ with transformation coefficients a_{up}^i. The index u refers to a spatial scale and the index p denotes a particular underlying factor at that scale

$$Z_i(\boldsymbol{x}) = \sum_{u=0}^{S} \sum_{p=1}^{N} a_{up}^i \, Y_p^u(\boldsymbol{x}) \tag{18}$$

For a given scale u_0 all factors $Y_p^{u_0}(\boldsymbol{x})$ have the same variogram $g_u(\boldsymbol{h})$. Formulated in this way, the linear model of coregionalization implies a nested multivariate variogram:

$$\boldsymbol{G}(\boldsymbol{h}) = \sum_{u=0}^{S} \boldsymbol{B}_u g_u(\boldsymbol{h}) \tag{19}$$

where $\boldsymbol{G}(\boldsymbol{h})$ is the matrix of variograms and the $\boldsymbol{B}_u$ are positive definite matrices of coefficients b_{ij}^u called *coregionalization matrices*. An efficient algorithm for fitting the nested multivariate variogram model to matrices of experimental direct and cross variograms, ensuring positive definite coregionalization matrices is given by Goulard and Voltz (1992).

Now, if the data are intrinsically correlated, what consequences does this have for the nested multivariate variogram and for the linear model of coregionalization?

When correlation is intrinsic, all coregionalization matrices are proportional to a basic matrix $\boldsymbol{B}$:

$$\boldsymbol{B}_u = a_u \boldsymbol{B} \tag{20}$$

and the nested multivariate variogram simplifies to:

$$\boldsymbol{G}(\boldsymbol{h}) = \boldsymbol{B} \sum_{u=0}^{S} a_u g_u(\boldsymbol{h}) = \boldsymbol{B}\gamma(\boldsymbol{h}) \tag{21}$$

which shows that the elements of the function matrix $\boldsymbol{G}(\boldsymbol{h})$ are all proportional to a basic variogram $\gamma(\boldsymbol{h})$.

In practice, the proportionality of the coregionalization matrices means that the eigenanalysis of each $\boldsymbol{B}_u$ will only differ in the eigenvalues, not in the eigenvectors. In other words, principal component analyses based on the coregionalization matrices will provide sets of factors combining the variables in the same way at the different spatial scales. Consequently, with intrinsic correlation the linear model reduces to:

$$Z_i(\boldsymbol{x}) = \sum_{p=1}^{N} a_p^i Y_p(\boldsymbol{x}) \tag{22}$$

with transformation coefficients a_p^i not depending on spatial scale and stemming from a classical MDA. The $Y_p(\boldsymbol{x})$ all have the same direct variogram $\gamma(\boldsymbol{h})$. The non-correlation between different $Y_p(\boldsymbol{x})$ implies that the cross variograms are zero. Thus the factors calculated from a classical MDA in presence of intrinsic correlation are autokrigeable.

Conversely, when the correlation is not intrinsic and the eigenvectors of different coregionalization matrices do not match, what happens if we perform a classical MDA on the data?

It can be seen from a relation between the variance-covariance matrix and the coregionalization matrices in the framework of a second-order stationary model without periodicities (Wackernagel, 1988):

$$\boldsymbol{V} = \sum_{u=0}^{S} \boldsymbol{B}_u \tag{23}$$

that the correlation structure described by the variance-covariance matrix $\boldsymbol{V}$ is a blending of the correlation structures at different spatial scales. A classical MDA based on $\boldsymbol{V}$ yields factors that are either just blurred or, in the worst case, completely meaningless.

This is illustrated in Fig. 1 by the cross variogram between the third and the fourth principal component from a classical MDA of gold exploration data (Wackernagel and Sanguinetti, 1992). In this example, the cross variogram for the two supposedly uncorrelated principal components PC3 and PC4 is not zero at short distances: a clear indication that correlation is not intrinsic.

CRITERIA FOR INTRINSIC CORRELATION

A first criterion is to use the *codispersion coefficients* $\mathrm{cc}_{ij}(\boldsymbol{h})$ (see Goovaerts, 1994 this issue) which is obtained by dividing the cross variograms by the square root of the corresponding product of direct variograms:

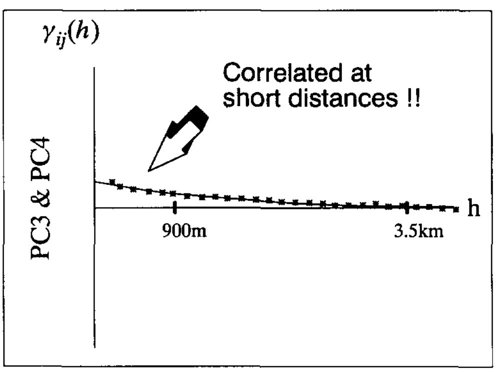

Fig. 1.

$$\mathrm{cc}_{ij}(\boldsymbol{h}) = \frac{\gamma_{ij}(\boldsymbol{h})}{\sqrt{\gamma_{ii}(\boldsymbol{h})\,\gamma_{jj}(\boldsymbol{h})}} \tag{24}$$

(i) if the codispersion coefficients are not equal to a constant independent of the lag $\boldsymbol{h}$, the correlation is not intrinsic (Matheron, 1965, p. 150).

It should be noted that the codispersion coefficient is in general not a criterion for autokrigeability, which can be checked by looking at graphs of *autokrigeability coefficients* $\mathrm{ac}_{i_0 j}(\boldsymbol{h})$ to see whether they can be assumed constant for a given pair (i_0, j):

$$\mathrm{ac}_{i_0 j}(\boldsymbol{h}) = \frac{\gamma_{i_0 j}(\boldsymbol{h})}{\gamma_{i_0 i_0}(\boldsymbol{h})} \tag{25}$$

A second procedure for identifying the presence/absence of intrinsic correlation, used by Wackernagel (1988), is to plot the position of the variables in the planes spanned by pairs of eigenvectors defining the most important factors and to compare these plots for different coregionalization matrices:

(ii) if the eigenanalysis of the coregionalization matrices yields similar systems of eigenvectors, the correlation can be assumed intrinsic.

The example illustrated by Fig. 1 exhibits a third criterion for intrinsic correlation:

(iii) if the factors computed from a classical principal component analysis have non zero cross variograms, the correlation between variables cannot be assumed intrinsic.

CONCLUSION

In this overview we have insisted upon the importance of coherence in the results of estimation when dealing with sums or linear combinations of variables in the isotopic case. Cokriging ensures the compatibility between an estimation of a sum and the separate estimation of each of its terms, while kriging generally does not.

In view of the additional computational and modeling effort implied by cokriging, it is important to know when cokriging is equivalent to kriging, i.e. when a variable is autokrigeable. This simplification occurs for ordinary (and simple) cokriging when the direct variogram of the variable of interest is proportional to the cross variograms with the auxiliary variables. A procedure for identifying this possible feature of the data is to examine the autokrigeability coefficients between the variable of interest and the auxiliary variables.

When the autokrigeability coefficients do not depend on the lag $\boldsymbol{h}$, the variable of interest is autokrigeable with respect to a given set of variables.

In regionalized MDA, linear combinations of variables need to be cokriged. Here the simplification to kriging takes place when the set of variables is intrinsically correlated, i.e. when each variable of the set is autokrigeable. A coregionalization analysis, establishing covariance matrices between variables at different spatial scales, will tell if the correlation coefficients are intrinsic, i.e. independent of spatial scale. The problem can also be approached from the other end, by performing first a classical principal component analysis neglegting the spatial relationships between the variables and then computing cross variograms between the principal components to see whether they are uncorrelated at all the spatial scales as they should be.

ACKNOWLEDGEMENTS

Thanks are due to Michel Grzebyk, Pierre Goovaerts, Paul Sampson, Jaap de Gruijter and an anonymous reviewer for helpful comments.

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